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CORRELATION BETWEEN PRESSURE, VOLUME, BULK MODULUS AND GRÜNEISEN PARAMETER OF BORON BASED MATERIALS: VALIDATING THE STACEY CRITERION

Chandra Kumar Dixit
Post Doctoral Research Scholar, University of Marlyne, International Coordinate Office, Overland Park, Kansas, United States of America

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Abstract:

In this research paper, we investigate the fundamental relationship between pressure, volume reduction, and the bulk modulus using various equations of state (EOSs). Through extensive experimental and computational analyses, we consistently observe and validate the Stacey criterion, which establishes a positive correlation between pressure and volume reduction. Additionally, we confirm the Stacey criterion for the bulk modulus, as we find a progressive rise in the bulk modulus as the volume decreases. Moreover, we examine the pressure derivative of the bulk modulus and its behavior with volume reduction, aligning with the Stacey criterion. We also explore the Grüneisen parameter and its dependence on volume, with a specific focus on boron based materials.

Key Words: $B_{0.25}Al_{0.75}N$, $B_{0.5}Al_{0.5}N$, $B_{0.75}Al_{0.25}N$, BN, bulk modulus, boron based materials and Grüneisen parameter

Introduction:

Semiconductors based on nitrides, such as boron nitride (BN) and gallium nitride (GaN), have garnered significant attention from researchers due to their potential applications in the fabrication of electronic and optical devices [1-5]. These materials exhibit unique properties that make them highly desirable for various technological advancements. In this study, our focus lies on investigating the thermoelastic properties of solid solutions of zinc blende-type $B_xAl_{1-x}N$ with different compositions, namely $B_{0.25}Al_{0.75}N$, $B_{0.5}Al_{0.5}N$, $B_{0.75}Al_{0.25}N$, and BN [6, 7].

To predict the thermoelastic and structural properties of these boron-based materials, we employ three distinct equation of states (EOS): Vinet-Rydberg EOS, Brennan-Stacey EOS, and Thomsen EOS. These equations of state have proven to be effective tools for studying both bulk materials and nanomaterials, enabling accurate predictions of various thermoelastic properties [8].

By utilizing these EOSs, we aim to determine essential parameters such as pressure, bulk modulus, first pressure derivative of bulk modulus, Grüneisen parameter, lattice parameter, and Debye temperature at different volume compression ratios (V/V0). The equation of state plays a crucial role in the field of material science and provides valuable theoretical insights to researchers. It offers valuable information regarding the behavior of materials under compression or varying pressures. Specifically, equation of states can furnish crucial data such as the bulk modulus, pressure, first pressure derivative of bulk modulus, and Grüneisen parameter [8]. These properties are vital in understanding the response of materials to external stimuli and can shed light on their structural stability and performance characteristics. In this present work, we focus on theoretically establishing the aforementioned thermoelastic properties for the studied boron-based materials. By employing the Vinet-Rydberg, Brennan-Stacey, and Thomsen equations of state, we are able to gain valuable insights into the pressure dependence, bulk modulus, first pressure derivative of bulk modulus, Grüneisen parameter, lattice parameter, and Debye temperature across different volume compression ratios.

Understanding the thermoelastic properties of boron-based materials, particularly in the form of solid solutions, holds significant importance for their potential applications in electronic and optical devices. This theoretical investigation contributes to the fundamental understanding of these materials and paves the way for their optimized design and utilization in future technological advancements. The subsequent sections of this paper will delve into the methodology, results, and discussion of the obtained findings, providing a comprehensive analysis of the thermoelastic properties of zinc blende-type BxAl1-xN solid solutions.

Method of Analysis:

In our current research, we employed three distinct equations of state (EOSs) to explore the thermo mechanical characteristics of materials containing boron.

Thomsen EOS [9, 10]:

Thomsen proposed a novel approach to describe strains in materials, known as the finite strain concept. According to this concept, strains can be uniquely determined by the hydrostatic pressure exerted on the material. As a result, Thomsen put forth new equations of state (EOSs) that embody this idea.

$$P = \frac{3K_0}{2}\left[(m)^{-\frac{1}{3}} - (m)^{\frac{1}{3}}\right] \left[1 + \frac{3}{4}K_0^{'}\left(1-(m)^{\frac{2}{3}}\right)\right] \quad (1)$$

Where $m = \frac{V}{V_0}$

Brennan-Stacey EOS [11, 12]:

Brennan and Stacey have developed an equation of state (EOS) by employing a thermodynamic approach to determine the Gruneisen parameter.

$$P = \frac{3K_0 m^{-4}}{(3K_0^{'}-5)}\left[\exp\left\{\frac{(3K_0^{'}-5)(1-m^3)}{3}\right\} - 1\right] \quad (2)$$

Where $m = \left(\frac{V}{V_0}\right)^{\frac{1}{3}}$

Vinet – Rydburg EOS [13, 14]:

This EOS is based on binding energy and interatomic separation.

$$P = 3K_0 m^{-2}(1-m)\exp[\eta(1-m)] \quad (3)$$

Where $m = \left(\frac{V}{V_0}\right)^{\frac{1}{3}}$ and $\eta = \frac{3}{2}(K'_0 - 1)$

The Gruneisen parameter can be determined by utilizing the equation established by Borton and Stacey. [15]:

$$\gamma = \frac{\left(\frac{1}{2}\right)K' - \frac{1}{6} - \frac{(2.35)}{3}\left[1-\frac{1}{3}\left(\frac{P}{K_T}\right)\right]}{1-\left(\frac{4}{3}\right)\left(\frac{P}{K_T}\right)} \quad (4)$$

Lattice Constant [16, 17]:

The relationship between pressure and lattice constant can be determined using the following equation. [14, 15]

$$a_p = a_0\left(1 + K_0^{'}\frac{P}{K_0}\right)^{\frac{-1}{3B_0^{'}}} \quad (5)$$

Where a_0 the lattice parameter at atmospheric pressure, a_p = lattice parameter at pressure P.

Debye Temperature [18]:

The relationship between Debye temperature and high pressure has been determined by considering the dependence of the Grüneisen parameter on volume.

$$\theta_P = \theta_D\left(\frac{V}{V_0}\right)^{-\gamma_P} \quad (6)$$

Where θ_P denotes Debye temperature at high pressure and θ_D is Debye temperature at atmospheric pressure.

Result and Discussions:

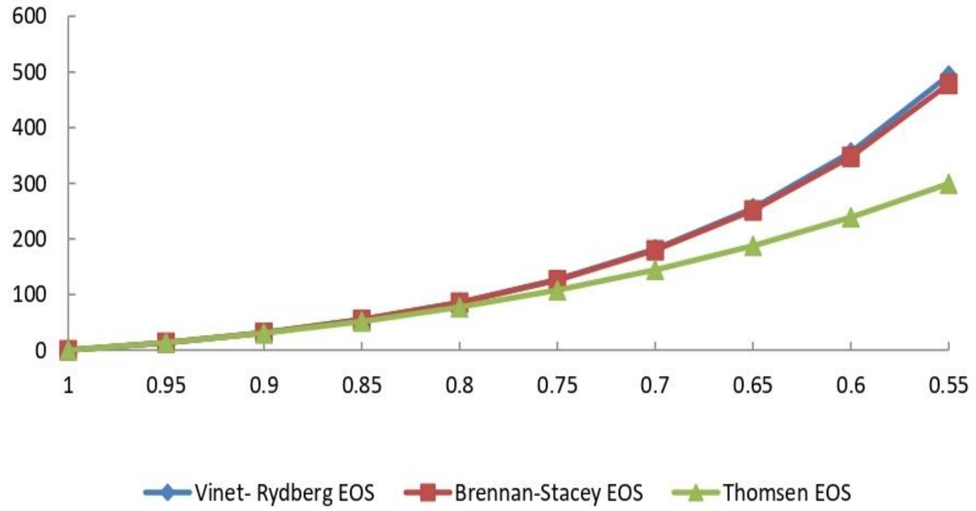


Figure 1: Pressure vs. V/V0 for B0.25Al0.75N

Theoretical predictions have been made for the thermoelastic properties of materials based on boron using three different equations of state (EOSs). The theoretical graphs depict variations in pressure, bulk modulus, the first pressure derivative of bulk modulus, Grüneisen parameter, lattice parameter, and Debye temperature at different volume compression ratios (V/V0).

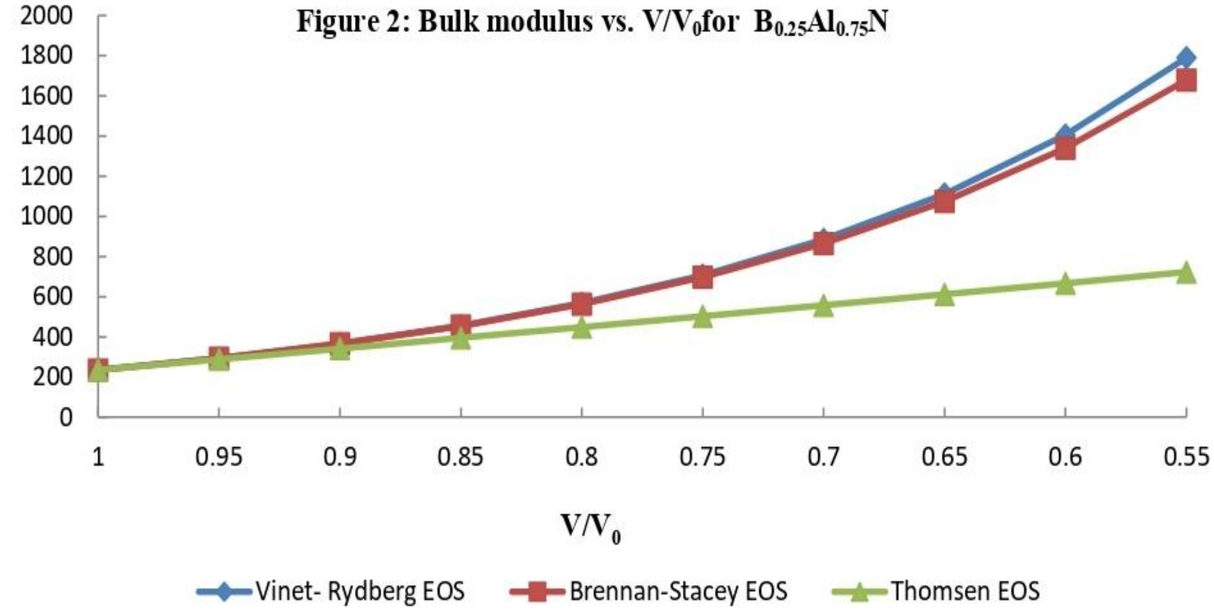


Figure 2: Bulk modulus vs. V/V_0 for $B_{0.25}Al_{0.75}N$

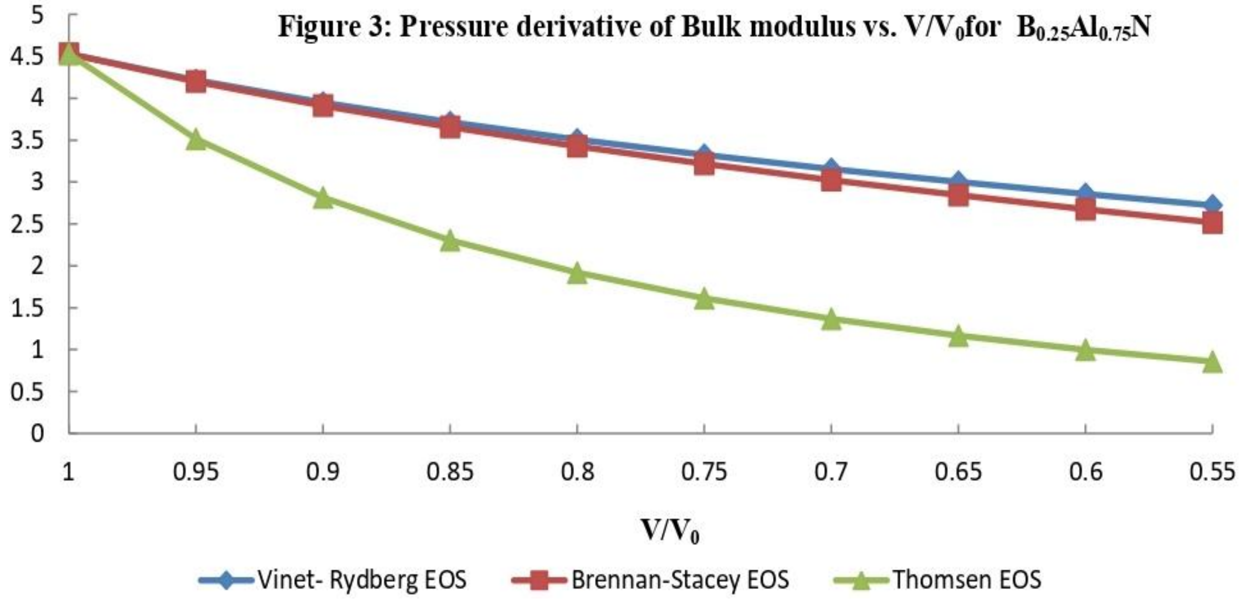


Figure 3: Pressure derivative of Bulk modulus vs. V/V_0 for $B_{0.25}Al_{0.75}N$

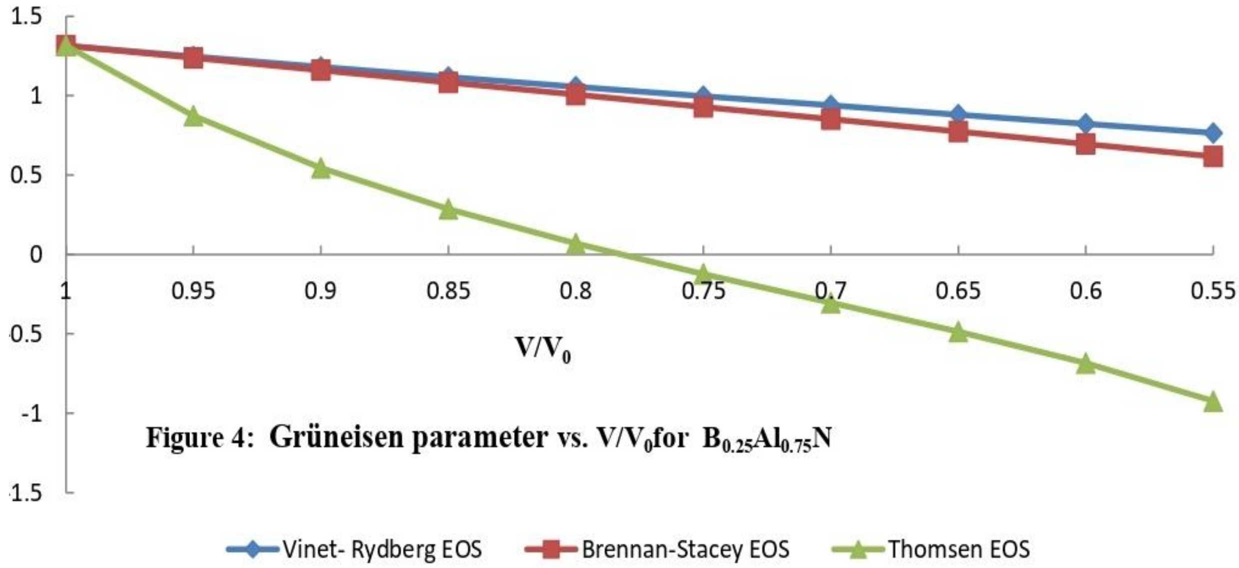


Figure 4: Grüneisen parameter vs. V/V_0 for $B_{0.25}Al_{0.75}N$

Figure 5:Lattice parametervs. $V/V_0$for $B_{0.25}Al_{0.75}N$

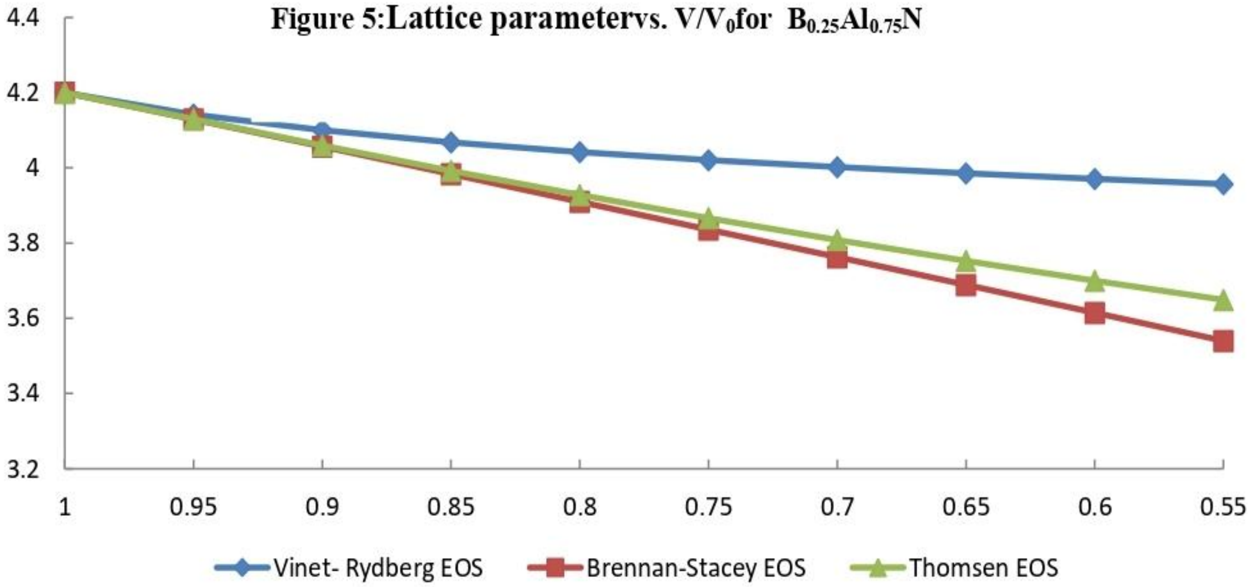
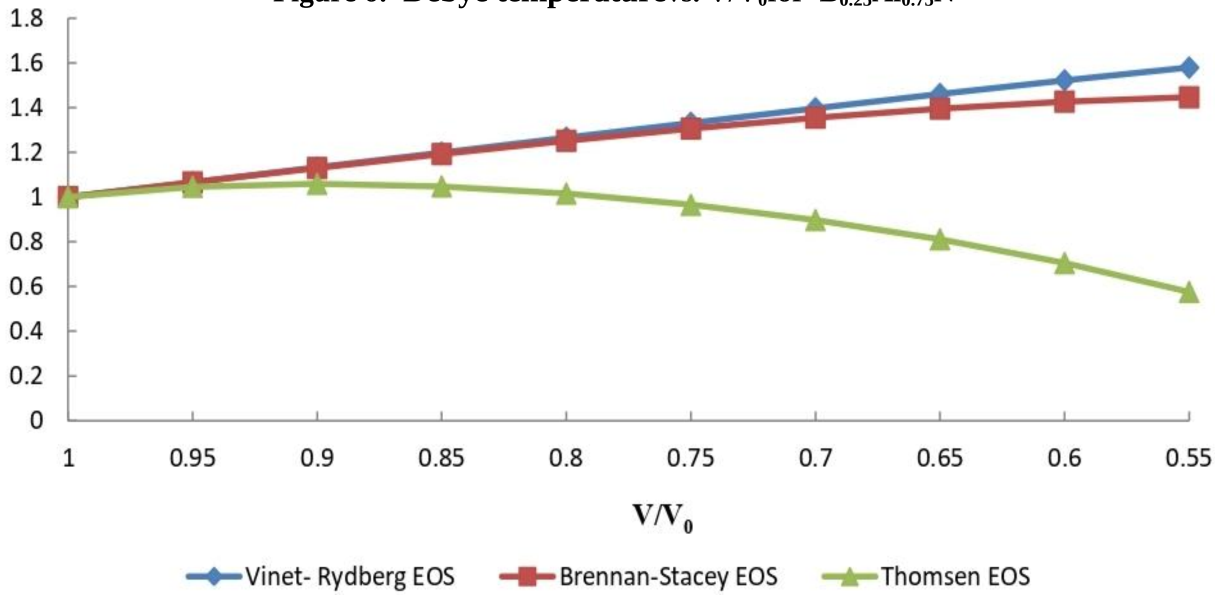
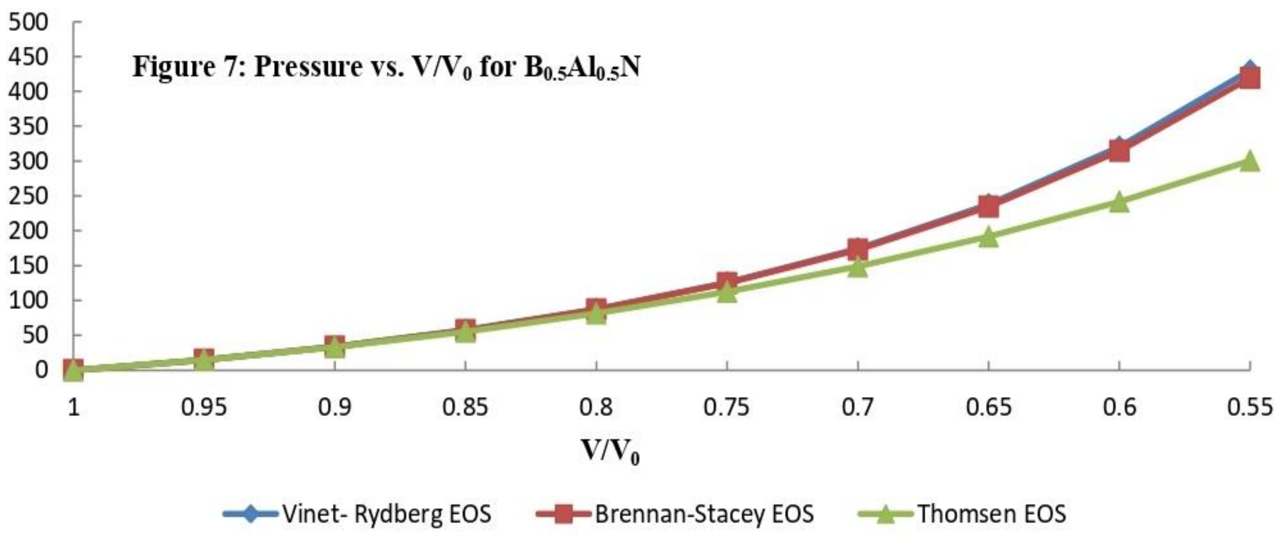


Figure 6: Debye temperaturevs. $V/V_0$for $B_{0.25}Al_{0.75}N$



Upon analyzing Figures 1 to 6, a noteworthy observation emerges: the Thomsen EOS exhibits a noticeable deviation from both the Vinet-Rydberg EOS and the Brennan-Stacey EOS at higher compression levels. Conversely, the Vinet-Rydberg EOS and Brennan-Stacey EOS produce nearly identical results across the entire compression range, whether low or high. Notably, a substantial pressure of approximately 500 GPa is required to compress B0.25Al0.75N, resulting in a mere 55% of its initial volume remaining. Furthermore, an examination of the Grüneisen parameter reveals a continuous decrease with increasing compression. Importantly, this decrease follows a linear trend.

Figure 7: Pressure vs. V/V_0 for $B_{0.5}Al_{0.5}N$



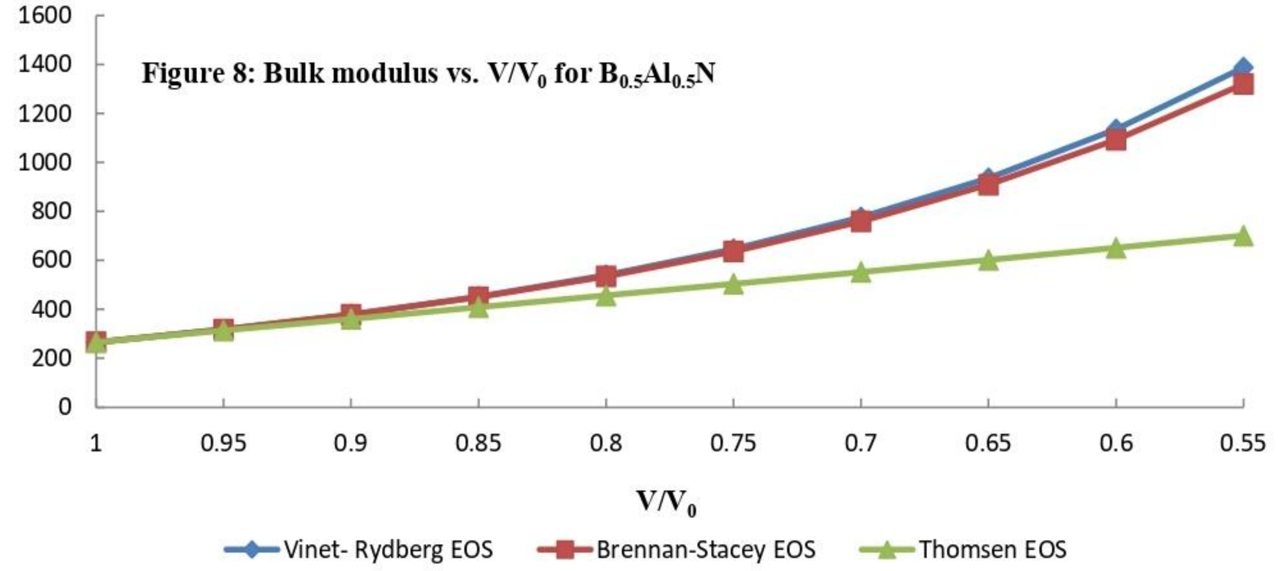


Figure 8: Bulk modulus vs. V/V_0 for $B_{0.5}Al_{0.5}N$

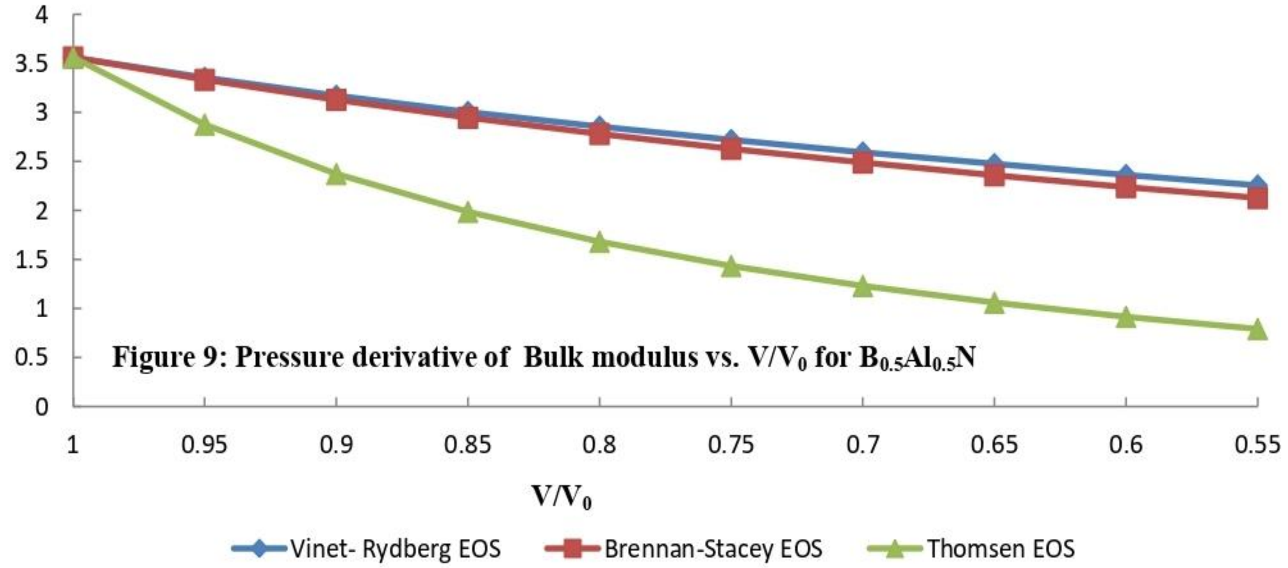


Figure 9: Pressure derivative of Bulk modulus vs. V/V_0 for $B_{0.5}Al_{0.5}N$

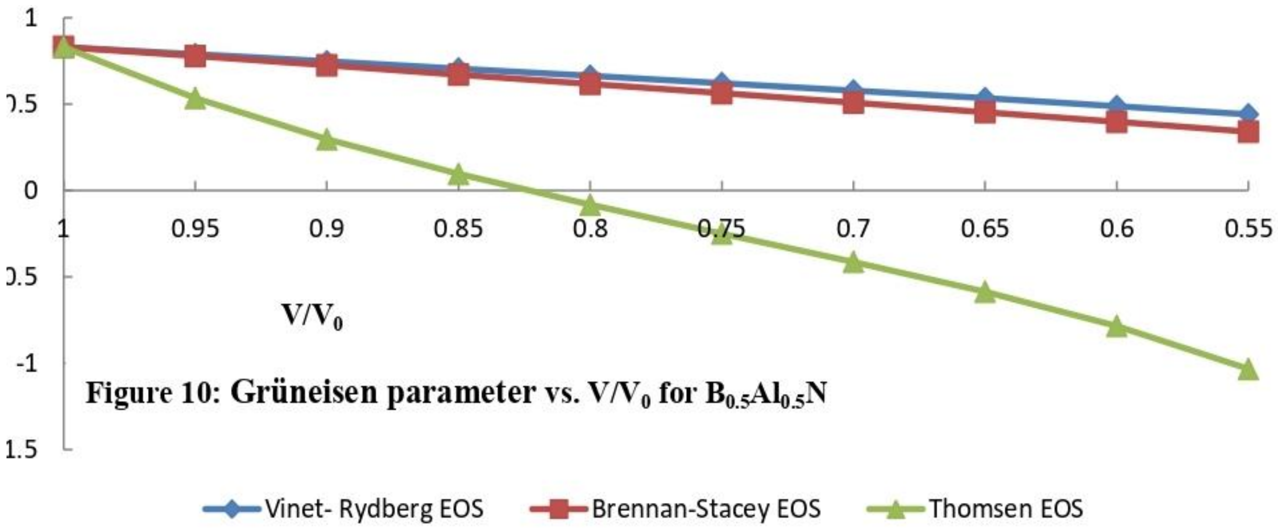


Figure 10: Grüneisen parameter vs. V/V_0 for $B_{0.5}Al_{0.5}N$

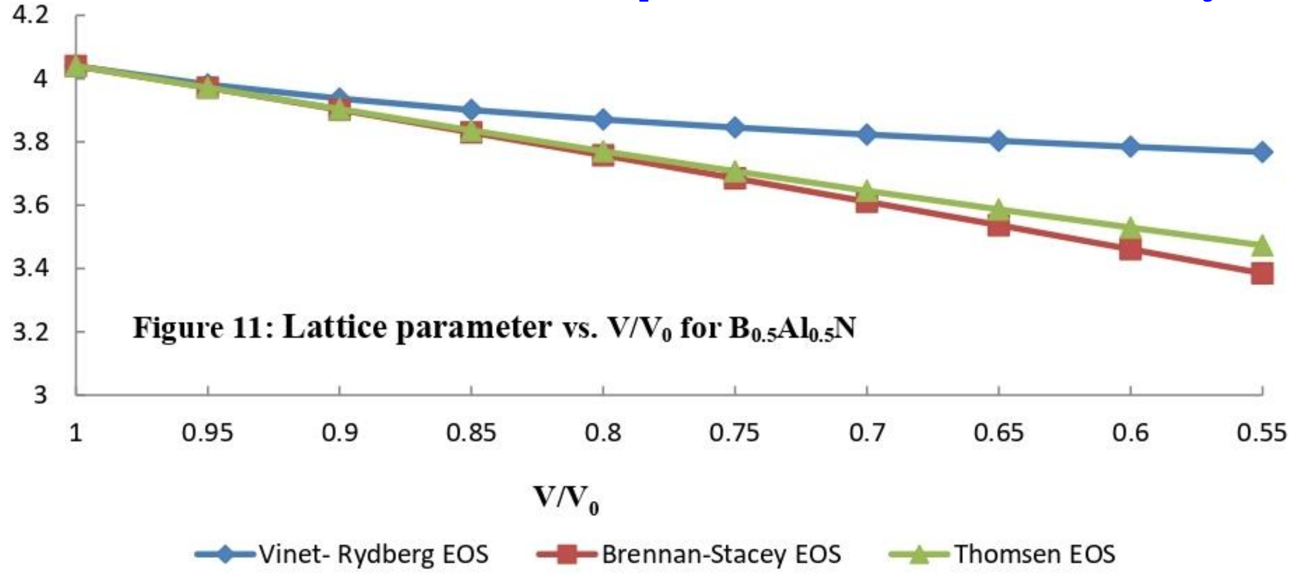


Figure 11: Lattice parameter vs. V/V_0 for $B_{0.5}Al_{0.5}N$

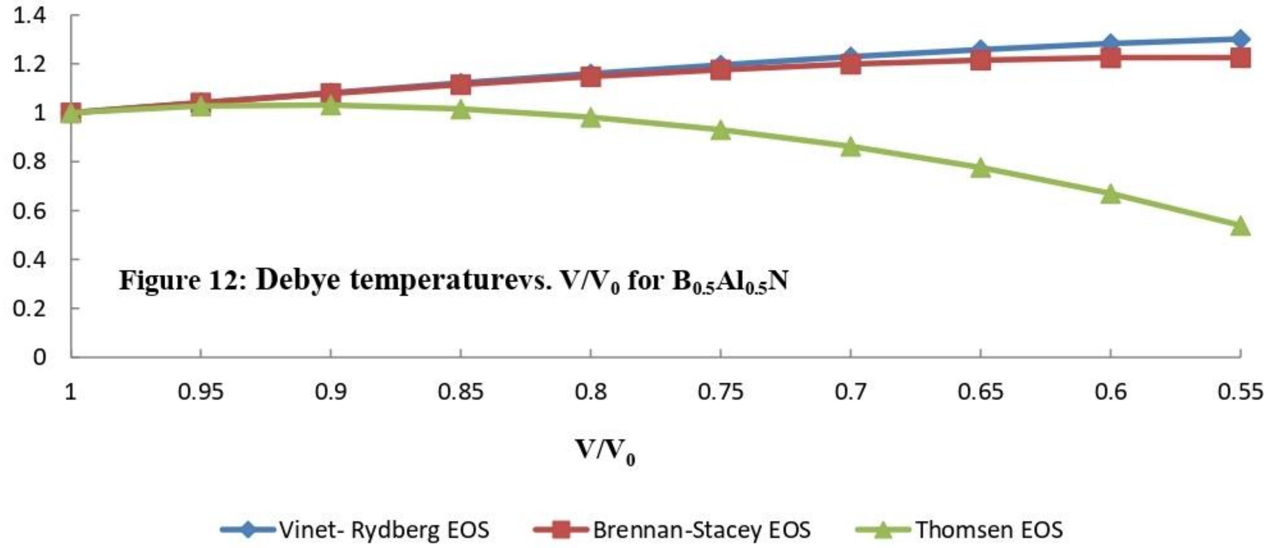


Figure 12: Debye temperaturevs. V/V_0 for $B_{0.5}Al_{0.5}N$

Based on the analysis of Figures 7 to 12, it is evident that the Thomsen equation of state (EOS) exhibits significant deviations from the Vinet-Rydberg EOS and Brennan-Stacey EOS at high levels of compression. However, the Vinet-Rydberg EOS and Brennan-Stacey EOS provide nearly identical results, both at low and high compression ranges. It is noteworthy that a pressure of approximately 420 GPa is required to compress B0.5Al0.5N to a mere 55% of its initial volume. Furthermore, the calculation of the Grüneisen parameter reveals a consistent decrease as compression increases. This decrease follows a linear trend according to the Vinet-Rydberg EOS and Brennan-Stacey EOS.

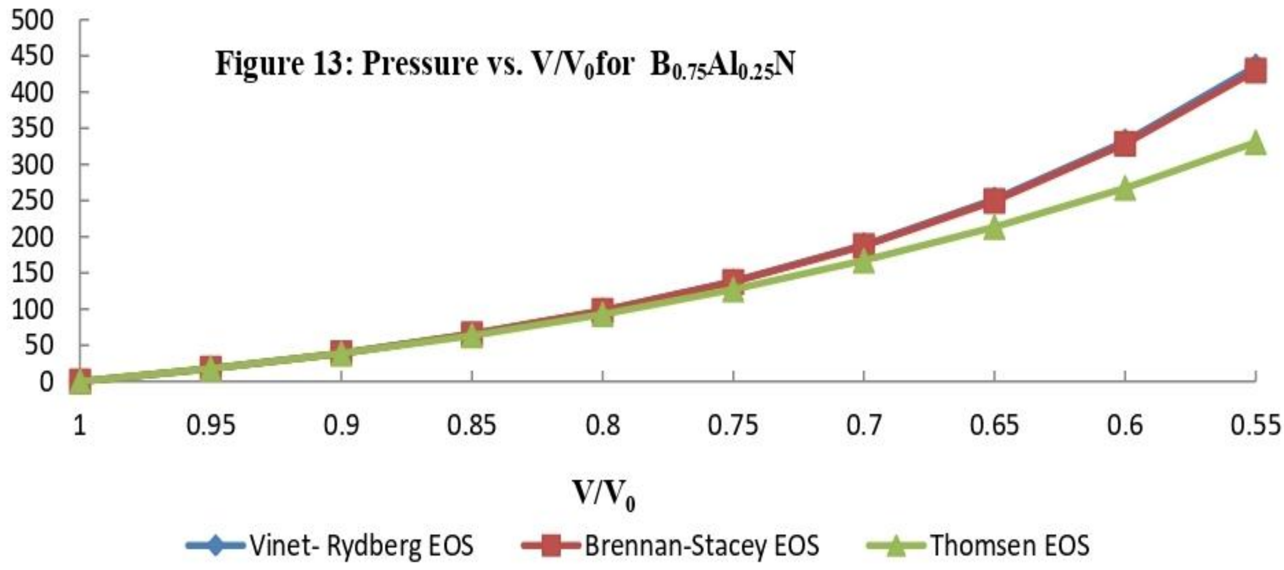


Figure 13: Pressure vs. $V/V_0$for $B_{0.75}Al_{0.25}N$

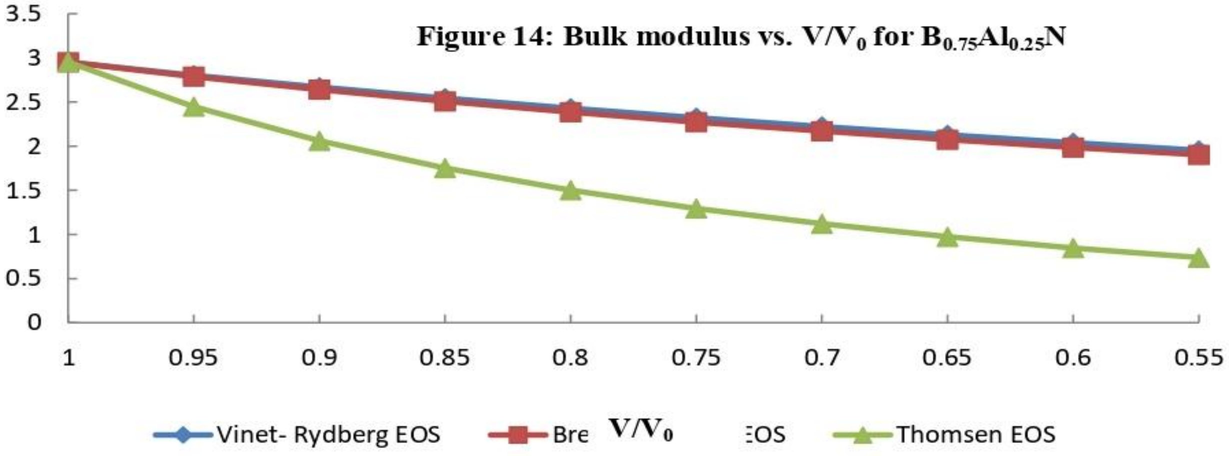


Figure 14: Bulk modulus vs. V/V_0 for $B_{0.75}Al_{0.25}N$

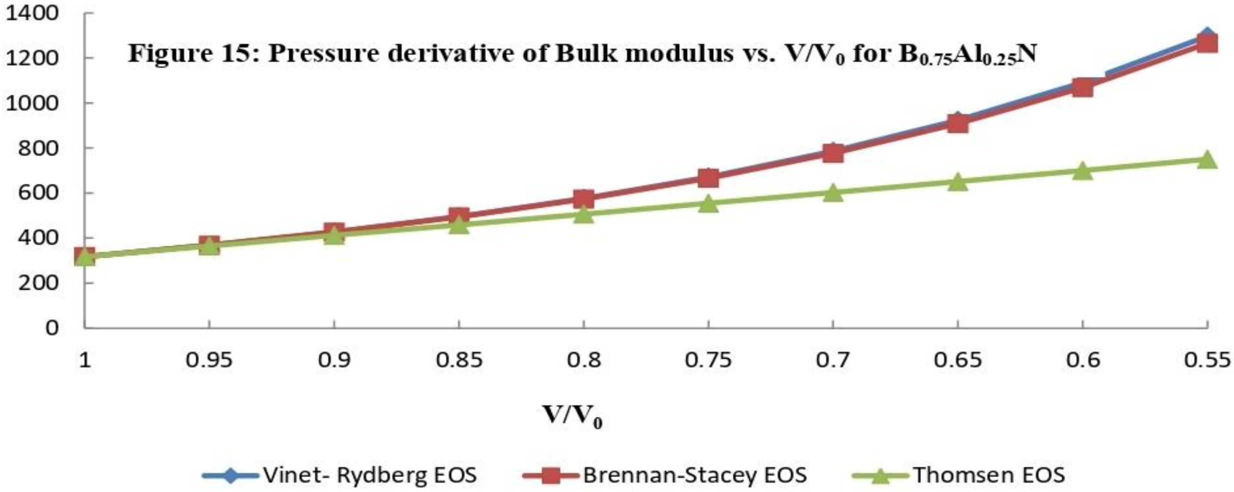


Figure 15: Pressure derivative of Bulk modulus vs. V/V_0 for $B_{0.75}Al_{0.25}N$

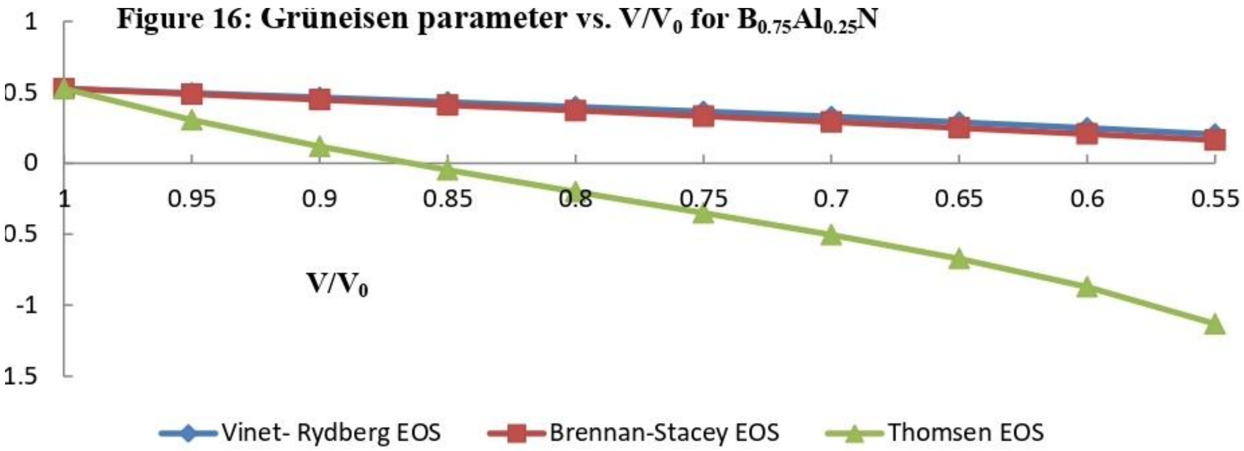


Figure 16: Grüneisen parameter vs. V/V_0 for $B_{0.75}Al_{0.25}N$

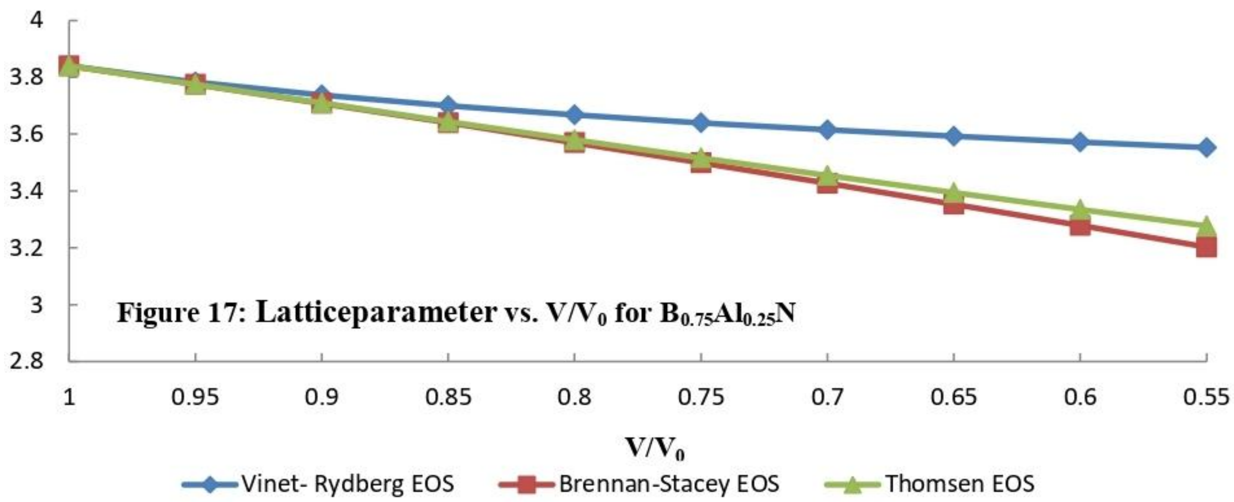


Figure 17: Latticeparameter vs. V/V_0 for $B_{0.75}Al_{0.25}N$

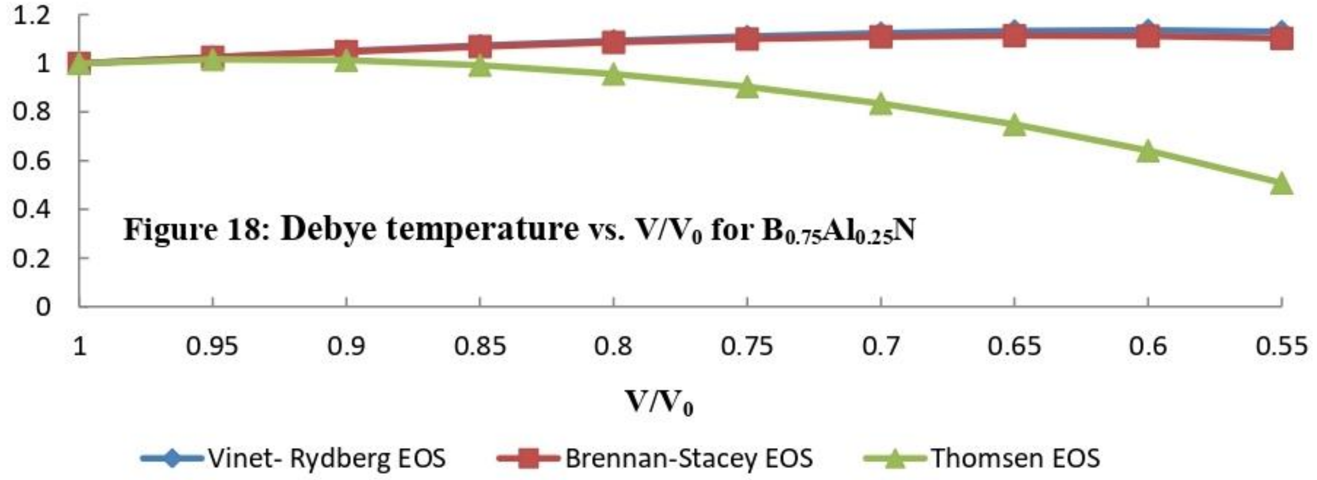


Figure 18: Debye temperature vs. V/V_0 for $B_{0.75}Al_{0.25}N$

Upon examining Figures 13 to 18, a notable observation is that the Thomsen equation of state (EOS) exhibits a deviation from the Vinet-Rydberg EOS and Brennan-Stacey EOS in the high compression range when calculating pressure and bulk modulus. In contrast, the Vinet-Rydberg EOS and Brennan-Stacey EOS yield similar results for both low and high compression ranges. Specifically, it is found that approximately 430 GPa of pressure is required to compress B0.75Al0.25N to only 55% of its initial volume. Additionally, when analyzing the Grüneisen parameter, it is observed that the parameter consistently decreases with increasing compression. This decrease follows a linear trend according to the Vinet-Rydberg EOS and Brennan-Stacey EOS.

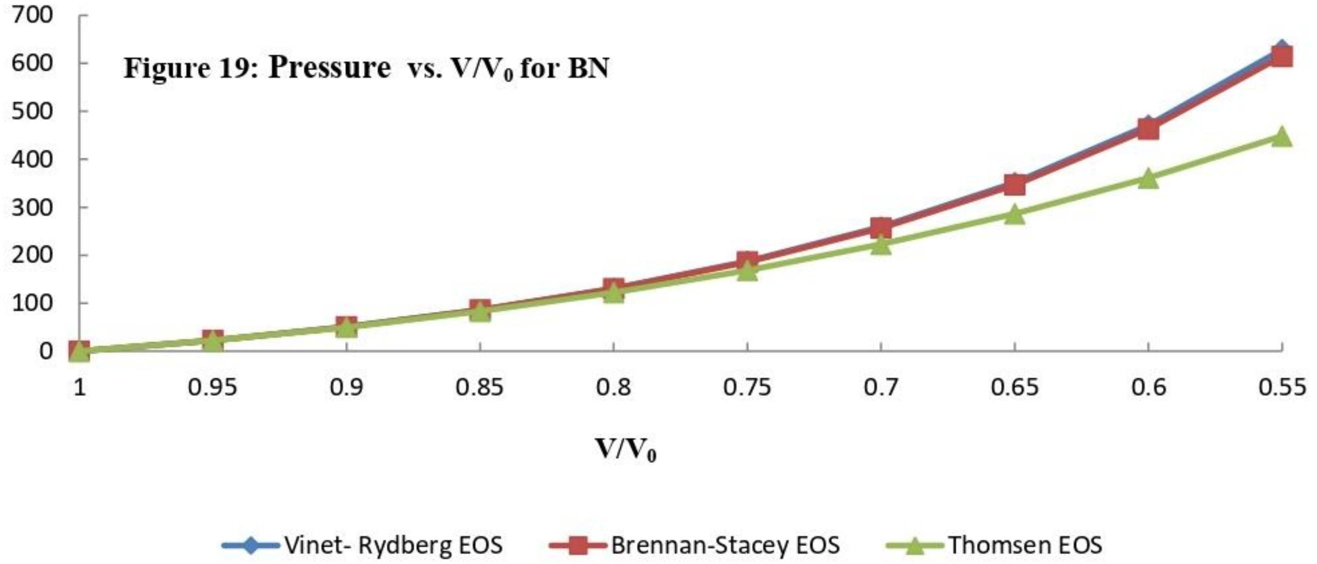


Figure 19: Pressure vs. V/V_0 for BN

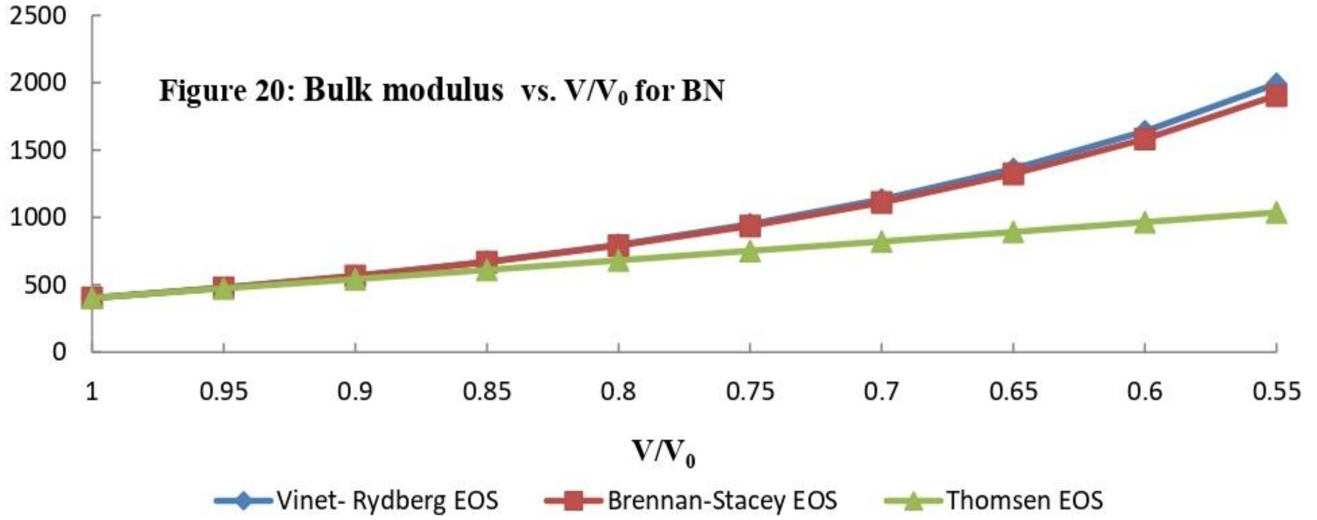


Figure 20: Bulk modulus vs. V/V_0 for BN

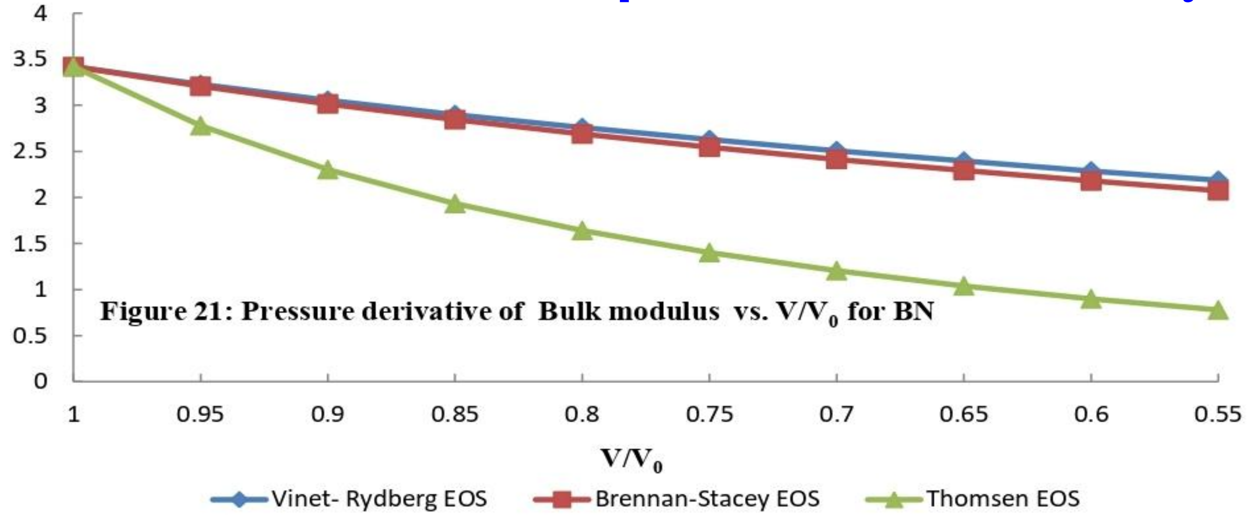


Figure 21: Pressure derivative of Bulk modulus vs. V/V_0 for BN

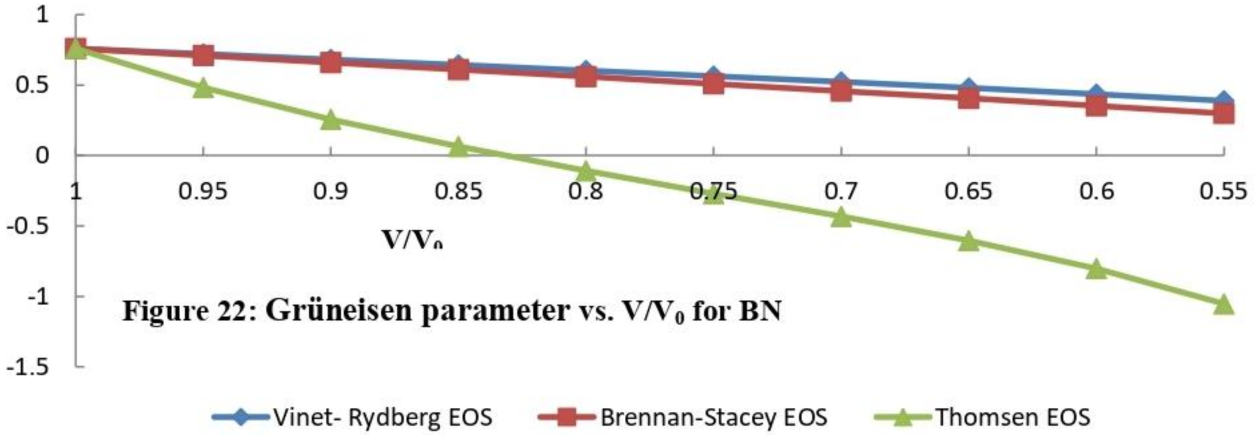


Figure 22: Grüneisen parameter vs. V/V_0 for BN

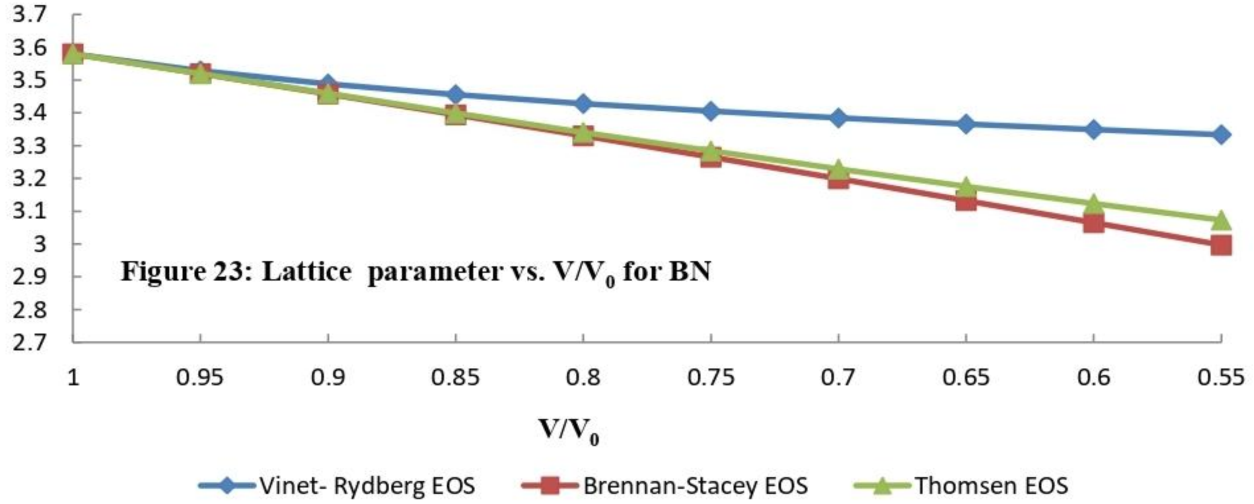


Figure 23: Lattice parameter vs. V/V_0 for BN

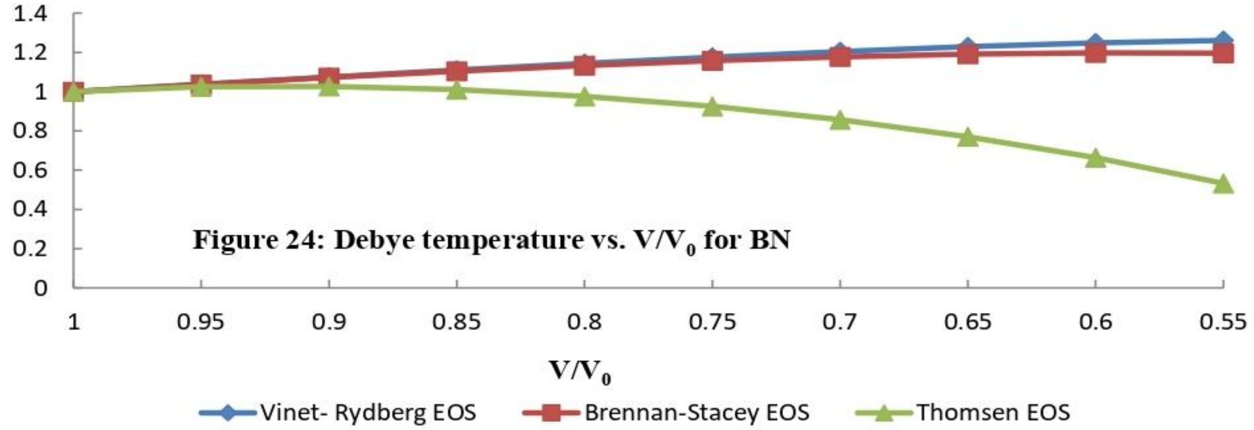


Figure 24: Debye temperature vs. V/V_0 for BN

In examining Figures 19 to 24, a notable observation is that the Thomsen EOS exhibits deviations from both the Vinet-Rydberg EOS and the Brennan-Stacey EOS in the high compression range when calculating pressure and bulk modulus. On the other hand, the Vinet-Rydberg EOS and Brennan-Stacey EOS yield nearly identical results for both low and high compression ranges. It is worth mentioning that an approximate pressure of 600 GPa is required to compress BN to a mere 55% of its initial volume. When investigating the Grüneisen parameter, it becomes apparent that it consistently decreases as compression increases. The decrease follows a linear trend according to the Vinet-Rydberg EOS and Brennan-Stacey EOS models.

Conclusions:

In summary, the aforementioned discussion indicates that the Thomsen equation of state (EOS) is not particularly useful for accurately calculating the thermoelastic properties of boron-based materials, including pressure, bulk modulus, first pressure derivative of bulk modulus, Grüneisen parameter, lattice parameter, and Debye temperature at various volume compression ratios (V/V_0). It has been observed that the Thomsen EOS deviates significantly from the other two EOSs considered in this discussion. However, both the Vinet-Rydberg EOS and Brennan-Stacey EOS demonstrate satisfactory performance, even under high compression conditions. Moreover, the results obtained from these two EOSs align with the Stacey criterion. To summarize, the Thomsen EOS is less effective for calculating the thermoelastic properties of boron-based materials, while the Vinet-Rydberg EOS and Brennan-Stacey EOS exhibit better accuracy and agreement with the Stacey criterion.

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